



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 01:04 PM GMT

PDB ID : 4J6L
Title : Crystal structure of calcium²⁺-free wild-type CD23 lectin domain (crystal form C)
Authors : Dhaliwal, B.; Yuan, D.; Sutton, B.J.
Deposited on : 2013-02-11
Resolution : 3.15 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

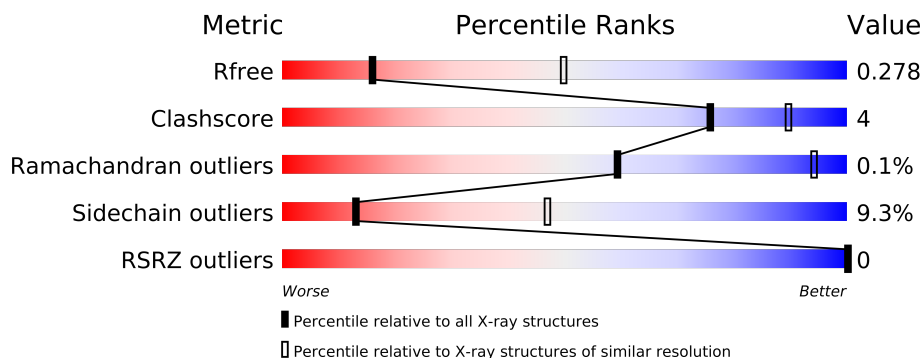
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.15 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1360 (3.22-3.10)
Clashscore	79885	1681 (3.22-3.10)
Ramachandran outliers	78287	1639 (3.22-3.10)
Sidechain outliers	78261	1638 (3.22-3.10)
RSRZ outliers	66119	1361 (3.22-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	143	
1	B	143	
1	C	143	
1	D	143	
1	E	143	
1	F	143	
1	G	143	
1	H	143	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8461 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Low affinity immunoglobulin epsilon Fc receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	133	Total	C	N	O	S	0	0	0
			1069	671	190	197	11			
1	B	133	Total	C	N	O	S	0	0	0
			1065	667	190	197	11			
1	C	132	Total	C	N	O	S	0	0	0
			1061	665	189	196	11			
1	D	133	Total	C	N	O	S	0	0	0
			1071	672	191	197	11			
1	E	130	Total	C	N	O	S	0	0	0
			1042	652	187	192	11			
1	F	128	Total	C	N	O	S	0	0	0
			1028	643	183	191	11			
1	G	135	Total	C	N	O	S	0	0	0
			1082	679	193	199	11			
1	H	129	Total	C	N	O	S	0	0	0
			1039	649	187	192	11			

- Molecule 2 is water.

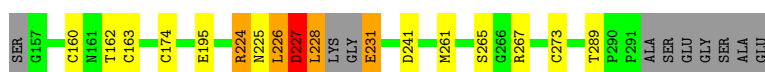
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	O	0	0
			1	1		
2	B	1	Total	O	0	0
			1	1		
2	D	1	Total	O	0	0
			1	1		
2	E	1	Total	O	0	0
			1	1		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Low affinity immunoglobulin epsilon Fc receptor

Chain A: 



- Molecule 1: Low affinity immunoglobulin epsilon Fc receptor

Chain B: 



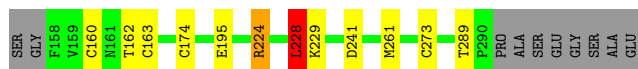
- Molecule 1: Low affinity immunoglobulin epsilon Fc receptor

Chain C: 



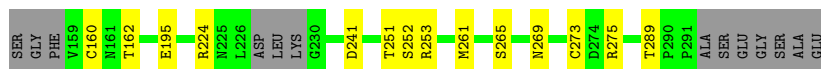
- Molecule 1: Low affinity immunoglobulin epsilon Fc receptor

Chain D: 



- Molecule 1: Low affinity immunoglobulin epsilon Fc receptor

Chain E: 



- Molecule 1: Low affinity immunoglobulin epsilon Fc receptor

Chain F: 



- Molecule 1: Low affinity immunoglobulin epsilon Fc receptor

Chain G: 



- Molecule 1: Low affinity immunoglobulin epsilon Fc receptor

Chain H: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	52.26Å 64.33Å 112.20Å 75.28° 82.39° 89.95°	Depositor
Resolution (Å)	49.36 – 3.15 49.35 – 3.15	Depositor EDS
% Data completeness (in resolution range)	96.5 (49.36-3.15) 96.7 (49.35-3.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 3.12Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.212 , 0.253 0.235 , 0.278	Depositor DCC
R_{free} test set	1193 reflections (5.37%)	DCC
Wilson B-factor (Å ²)	49.5	Xtriage
Anisotropy	0.494	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.3	EDS
Estimated twinning fraction	0.066 for -h,k,k-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 23393 reflections	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	8461	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.50	0/1102	0.82	3/1493 (0.2%)
1	B	0.50	0/1098	0.71	0/1487
1	C	0.47	0/1094	0.68	0/1482
1	D	0.51	0/1104	0.73	1/1495 (0.1%)
1	E	0.51	0/1074	0.73	0/1455
1	F	0.61	0/1058	0.80	2/1430 (0.1%)
1	G	0.51	0/1116	0.79	2/1512 (0.1%)
1	H	0.50	0/1070	0.83	1/1447 (0.1%)
All	All	0.52	0/8716	0.76	9/11801 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	H	0	1
All	All	0	2

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	255	GLN	CB-CA-C	13.51	137.43	110.40
1	A	227	ASP	CB-CA-C	11.77	133.94	110.40
1	G	231	GLU	N-CA-C	9.61	136.94	111.00
1	A	227	ASP	N-CA-C	-8.06	89.23	111.00
1	A	227	ASP	C-N-CA	-6.08	106.51	121.70
1	F	254	SER	C-N-CA	5.66	135.86	121.70
1	F	231	GLU	N-CA-C	5.64	126.22	111.00
1	G	231	GLU	CB-CA-C	-5.18	100.05	110.40
1	D	228	LEU	N-CA-C	-5.02	97.44	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	227	ASP	Peptide
1	H	255	GLN	Peptide

5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1069	0	0	11	3
1	B	1065	0	0	2	0
1	C	1061	0	0	1	0
1	D	1071	0	0	5	0
1	E	1042	0	0	0	0
1	F	1028	0	0	4	0
1	G	1082	0	0	1	1
1	H	1039	0	0	9	4
2	A	1	0	0	0	0
2	B	1	0	0	1	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
All	All	8461	0	0	31	4

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (31) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:226:LEU:N	1:A:226:LEU:CD2	2.32	0.93
1:A:227:ASP:CA	1:A:228:LEU:C	2.35	0.90
1:H:253:ARG:O	1:H:255:GLN:N	2.05	0.90
1:A:228:LEU:N	1:A:228:LEU:CD1	2.34	0.89
1:H:252:SER:O	1:H:253:ARG:CG	2.30	0.79
1:D:228:LEU:O	1:D:229:LYS:CB	2.30	0.78
1:A:227:ASP:C	1:A:228:LEU:CD1	2.64	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:165:GLU:OE2	2:B:301:HOH:O	2.13	0.66
1:A:225:ASN:OD1	1:A:226:LEU:N	2.29	0.66
1:A:227:ASP:O	1:A:228:LEU:CD1	2.45	0.65
1:H:253:ARG:C	1:H:254:SER:OG	2.30	0.62
1:A:228:LEU:CD2	1:A:231:GLU:CG	2.78	0.61
1:F:231:GLU:CG	1:F:231:GLU:O	2.47	0.61
1:A:228:LEU:CD2	1:A:231:GLU:CB	2.79	0.60
1:B:274:ASP:OD2	1:D:224:ARG:NH2	2.36	0.58
1:D:229:LYS:CE	1:F:254:SER:N	2.67	0.57
1:A:227:ASP:N	1:A:228:LEU:C	2.63	0.51
1:C:163:CYS:SG	1:C:174:CYS:SG	3.08	0.51
1:H:251:THR:OG1	1:H:251:THR:O	2.30	0.50
1:F:225:ASN:OD1	1:F:230:GLY:O	2.31	0.49
1:H:253:ARG:O	1:H:254:SER:OG	2.35	0.44
1:H:253:ARG:O	1:H:254:SER:CB	2.61	0.44
1:H:252:SER:C	1:H:253:ARG:CG	2.85	0.44
1:A:163:CYS:SG	1:A:174:CYS:SG	3.16	0.44
1:A:224:ARG:CG	1:A:225:ASN:N	2.82	0.43
1:H:253:ARG:O	1:H:255:GLN:O	2.37	0.42
1:F:259:CYS:SG	1:F:273:CYS:SG	3.17	0.42
1:D:163:CYS:SG	1:D:174:CYS:SG	3.19	0.41
1:D:228:LEU:O	1:D:229:LYS:CG	2.69	0.41
1:G:225:ASN:OD1	1:G:230:GLY:O	2.38	0.40
1:H:163:CYS:SG	1:H:174:CYS:SG	3.20	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:267:ARG:NH1	1:H:254:SER:O[1_655]	1.69	0.51
1:A:267:ARG:CZ	1:H:254:SER:O[1_655]	1.81	0.39
1:A:267:ARG:NH2	1:H:254:SER:O[1_655]	1.83	0.37
1:G:231:GLU:OE1	1:H:251:THR:CG2[1_655]	2.06	0.14

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	129/143 (90%)	121 (94%)	8 (6%)	0	100	100
1	B	129/143 (90%)	120 (93%)	9 (7%)	0	100	100
1	C	128/143 (90%)	120 (94%)	8 (6%)	0	100	100
1	D	131/143 (92%)	120 (92%)	11 (8%)	0	100	100
1	E	126/143 (88%)	120 (95%)	6 (5%)	0	100	100
1	F	124/143 (87%)	114 (92%)	9 (7%)	1 (1%)	27	77
1	G	133/143 (93%)	121 (91%)	12 (9%)	0	100	100
1	H	127/143 (89%)	117 (92%)	10 (8%)	0	100	100
All	All	1027/1144 (90%)	953 (93%)	73 (7%)	1 (0%)	59	94

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	161	ASN

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	114/120 (95%)	101 (89%)	13 (11%)	8	35
1	B	113/120 (94%)	101 (89%)	12 (11%)	10	38
1	C	113/120 (94%)	101 (89%)	12 (11%)	10	38
1	D	114/120 (95%)	105 (92%)	9 (8%)	18	58
1	E	111/120 (92%)	97 (87%)	14 (13%)	7	28
1	F	109/120 (91%)	101 (93%)	8 (7%)	20	63
1	G	115/120 (96%)	107 (93%)	8 (7%)	21	65
1	H	110/120 (92%)	102 (93%)	8 (7%)	20	63
All	All	899/960 (94%)	815 (91%)	84 (9%)	13	47

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	160	CYS
1	A	162	THR
1	A	195	GLU
1	A	224	ARG
1	A	226	LEU
1	A	227	ASP
1	A	228	LEU
1	A	231	GLU
1	A	241	ASP
1	A	261	MET
1	A	265	SER
1	A	273	CYS
1	A	289	THR
1	B	160	CYS
1	B	162	THR
1	B	165	GLU
1	B	195	GLU
1	B	216	HIS
1	B	224	ARG
1	B	241	ASP
1	B	261	MET
1	B	265	SER
1	B	273	CYS
1	B	285	LEU
1	B	289	THR
1	C	160	CYS
1	C	162	THR
1	C	165	GLU
1	C	195	GLU
1	C	226	LEU
1	C	241	ASP
1	C	253	ARG
1	C	261	MET
1	C	263	ARG
1	C	265	SER
1	C	273	CYS
1	C	289	THR
1	D	160	CYS
1	D	162	THR
1	D	195	GLU
1	D	224	ARG
1	D	228	LEU
1	D	241	ASP

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Mol	Chain	Res	Type
1	D	261	MET
1	D	273	CYS
1	D	289	THR
1	E	160	CYS
1	E	162	THR
1	E	195	GLU
1	E	224	ARG
1	E	241	ASP
1	E	251	THR
1	E	252	SER
1	E	253	ARG
1	E	261	MET
1	E	265	SER
1	E	269	ASN
1	E	273	CYS
1	E	275	ARG
1	E	289	THR
1	F	192	ASP
1	F	195	GLU
1	F	197	GLN
1	F	229	LYS
1	F	241	ASP
1	F	255	GLN
1	F	261	MET
1	F	282	CYS
1	G	160	CYS
1	G	165	GLU
1	G	195	GLU
1	G	241	ASP
1	G	261	MET
1	G	265	SER
1	G	273	CYS
1	G	289	THR
1	H	195	GLU
1	H	229	LYS
1	H	241	ASP
1	H	251	THR
1	H	254	SER
1	H	261	MET
1	H	265	SER
1	H	273	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no

such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	133/143 (93%)	-0.05	0 100 100	27, 49, 80, 98	0
1	B	133/143 (93%)	-0.04	0 100 100	28, 48, 84, 105	0
1	C	132/143 (92%)	-0.06	0 100 100	31, 50, 82, 96	0
1	D	133/143 (93%)	-0.01	0 100 100	35, 58, 87, 101	0
1	E	130/143 (90%)	-0.00	0 100 100	28, 49, 79, 108	0
1	F	128/143 (89%)	-0.01	0 100 100	35, 58, 85, 106	0
1	G	135/143 (94%)	-0.00	0 100 100	38, 57, 86, 98	0
1	H	129/143 (90%)	-0.01	0 100 100	32, 57, 90, 111	0
All	All	1053/1144 (92%)	-0.02	0 100 100	27, 54, 85, 111	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.